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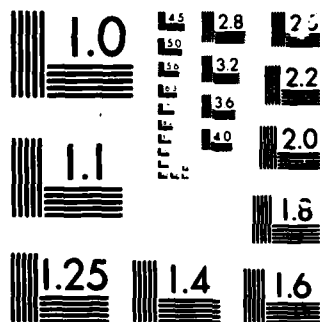
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QUANTITATIVE MODELING OF GROWTH AND DISPERSAL IN POPULATION MODELS*

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ABSTRACT

We discuss techniques for the estimation of nonlinearities and state-dependent coefficients in parabolic partial differential equations. Applications to density-dependent population dispersal and nonlinear growth/predation models are presented. Computational results using parallel and vector architectures are discussed.

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INTRODUCTION

In this presentation we discuss methods for inverse or parameter estimation problems which can be employed as quantitative modeling techniques in models for distributed (spatially, age, size, etc.) biological systems. In this context they may be useful in attempts to understand, elaborate on, or further refine details of specific mechanisms for dispersal, growth, interaction, etc. in wide classes of models. We have also used these techniques in a number of biologically related problems [1] such as bioturbation [12], [14], [15] and climatology [19]. In addition to an overview of ideas underlying these techniques, we shall present here brief discussions and some findings on two specific biological problems for which we are currently using them successfully.

A typical inverse problem entails some given or hypothesized dynamical model with "parameters" q (often temporally and/or "spatially" or even state dependent) and "states" $u(t,x;q)$, $0 \leq t \leq T$, $x \in \Omega$, which depend on the parameters through a dynamical system of equations. One has observations or data \hat{u}_{ij} for $u(t_i, x_j; q)$ and wishes to choose, from some admissible parameter set Q , parameters \bar{q} so as to give a best fit of the model to the data. For example, we might have a hypothesized model for transport

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left[V(t,x,u)u \right] = \frac{\partial}{\partial x} \left[D(t,x,u) \frac{\partial u}{\partial x} \right] + F(t,x,u) \quad (1)$$

with initial and boundary conditions also possibly depending on the unknown parameters $q = (V, D, F)$. Given data \hat{u}_{ij} , we seek to minimize a fit-to-data criterion such as a least-squares

$$J(q) = \sum_{i,j} |u(t_i, x_j; q) - \hat{u}_{ij}|^2 \quad (2)$$

over a specified class Q of functions (V, D, F) so as to obtain a best estimate $\bar{q} = (\bar{V}, \bar{D}, \bar{F})$. In addition to obtaining estimates for q , usually one desires to analyze in some way the "goodness" of the model in describing the phenomena one is modeling. We shall elaborate on some related questions in this regard below.

The methods we discuss briefly here can be powerful modeling tools when carefully and correctly used. Some of the novel features of our recent efforts include the capabilities for estimation of (i) state or density dependent dispersal coefficients such as D above in (1), (ii) system nonlinearities such as F in (1), and (iii) boundary parameters in both simple and not-so-simple boundary conditions (we give an example in the discussions on size dependent models below). Furthermore, there are a number of modeling related questions that one might hope to address from a theoretical or computational (or both) viewpoint with the aid of these techniques. These include:

- (a) Experimental design [3], [4], [5]: What is the appropriate data required to support analysis of a particular model or mechanism? E.g., How many time vs. spatial observations must be made, or what type of initial data is needed to study movement patterns?
- (b) Robustness of model parameters [1], [3], [8], [16], [19]: Do the problem formulation and the methods enjoy certain stability properties? E.g., Do the parameter estimates and the estimation methods depend continuously on observation noise, initial data, amounts of data available, problem constraints, etc.?
- (c) Identifiability [18], [25]: Is the map from the parameter space to the observation sufficiently well-behaved so that the methods can produce unique estimates?
- (d) Model comparison [3], [5], [19]: Can one make evaluations regarding the importance and type of mechanisms needed to model given phenomena? E.g., Which is more important in particular transport phenomena: convection, diffusion, nonlinear effects, dynamic (time varying) vs. heterogeneous (spatially varying) terms or coefficients? What level of refinement in modeling terms can be supported by the experimental design and data? Do model refinements yield statistically significant improvements in explanation of the data?

CONCEPTUAL CONSIDERATIONS

We next outline briefly certain ideas related to the problems and methods that are the focus of this presentation. At the same time we shall indicate some questions that may arise in either theoretical or computational aspects of investigations using the methods. These discussions can be made precise and mathematically rigorous, but for the sake of brevity, we shall not do that here.

For the purposes of illustration, we return to the problem of minimizing the functional of (2) subject to the system (1) relating the states and parameters. Such problems lead to the need for optimization techniques for constrained problems that are infinite dimensional in nature. One has a system with states $(t,x) \rightarrow u(t,x)$ in some infinite dimensional function space X and parameters $(t,x) \rightarrow q(t,x)$, or $(t,x,u) \rightarrow q(t,x,u)$ if the parameters are state dependent, in some infinite dimensional function space Q . These problems can be concisely stated in a theoretical framework using either the theory of semigroups or evolution operators, or the theory of sesquilinear forms in Hilbert spaces. We won't pursue the details here, but refer the reader to [2], [7], [9], [13], [15].

In any case, this leads to the recognition that in order to effectively develop computational techniques, one must introduce approximation schemes for the state and

parameter spaces. That is, one needs families of finite dimensional spaces X^N and Q^M (such as finite elements, splines, spectral families) such that X^N approximates X well as $N \rightarrow \infty$ and Q^M approximates Q as $M \rightarrow \infty$. (We shall (imprecisely) write this as $X^N \rightarrow X$, $Q^M \rightarrow Q$ or simply $N \rightarrow \infty$, $M \rightarrow \infty$, in the discussions below.) One then must develop schemes to solve the approximate problems obtained when u in J of (2) is replaced by the approximate states $u^N \in X^N$ satisfying some equation approximating (1). Minimization is carried out over Q^M yielding approximate best-fit parameters $\bar{q}^{N,M}$. Thus, the algorithms we have developed and used (e.g. see [3], [5], [8] for details) entail iterative optimization techniques combined with appropriately chosen approximation schemes based on families X^N , Q^M .

Among the important questions associated with these approximation ideas are those of method convergence and method stability. In the first, one must argue that $\bar{q}^{N,M} \rightarrow \bar{q}$ as $X^N \rightarrow X$, $Q^M \rightarrow Q$, where \bar{q} is a solution to the original problem involving (1) and (2). That is, one must assure fidelity of the estimates under sufficiently accurate approximation of state and parameter spaces. The concept of stability is related to a continuous dependence of the estimates on the observed data, X^N , and Q^M . More precisely, if $\bar{q}^{N,M}(\hat{u})$ denotes solutions to the approximate problems corresponding to state space X^N , parameter space Q^M and data \hat{u} , and if (\hat{u}^K) is a sequence of data with $\hat{u}^K \rightarrow \hat{u}$, then one desires to guarantee that $\bar{q}^{N,M}(\hat{u}^K) \rightarrow \bar{q}(\hat{u})$ as $N, M, K \rightarrow \infty$, where $\bar{q}(\hat{u})$ is a solution of the original problem with data \hat{u} . That is, fidelity of the estimates will hold with sufficiently small noise in the observations as well as sufficiently accurate approximations of the state and parameter spaces. For further discussions see [1], [18].

One can develop a general theory to guarantee theoretically and computationally well-behaved algorithms based on the ideas we have used in a wide class of problems including the examples discussed below. The arguments rely heavily on ideas from functional analysis, approximation theory and compactness. We refer the reader to [1], [4], [8], [15], [18], [25] for further elaboration and details. We only note here that fundamental to all these convergence and stability results is the establishment that $u^N(t, x; q^M) \rightarrow u(t, x; q)$ in some sense (i.e., in an appropriate X -topology) whenever $q^M \rightarrow q$ in an appropriate sense (i.e., in a Q -topology). For further discussion of mathematical ideas, and implementation and testing of the methods, we refer to the presentations in [3], [5] in addition to those references cited above. Here we discuss several projects in which these methods are playing a fundamental role and outline some new results in two areas.

INSECT DISPERSAL/GROWTH MODELS

We have, in collaboration with P. Kareiva (U. Washington), considered a number of aspects of insect movement and growth. In several cases our quantitative methods have proved useful in planning the experiments as well as actually investigating various models. Among the investigations we have pursued are:

- (i) quantifying "initial disturbance" effects in dispersal rates for flea beetle movement in mark-recapture experiments in cultivated collard patches [3], [5], [21], [22], [23];
- (ii) studying the effects of density-dependent dispersal rates, nonlinear growth, interaction, and predation in multiple species models such as those for ladybug-aphid-goldenrod

experiments [10], [24];

- (iii) quantifying "preferred direction" components in cabbage root fly movement in two-dimensional domains [6], [31].

In regard to the investigations of (ii), we note that the methods can be used effectively to estimate the shape of density-dependent dispersal coefficients D and nonlinear growth terms f in models of the form

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left[D(t, x, u) \frac{\partial u}{\partial x} \right] + f(u) \quad (3)$$

where $D(t, x, \cdot)$ has the form depicted in Figure 1.

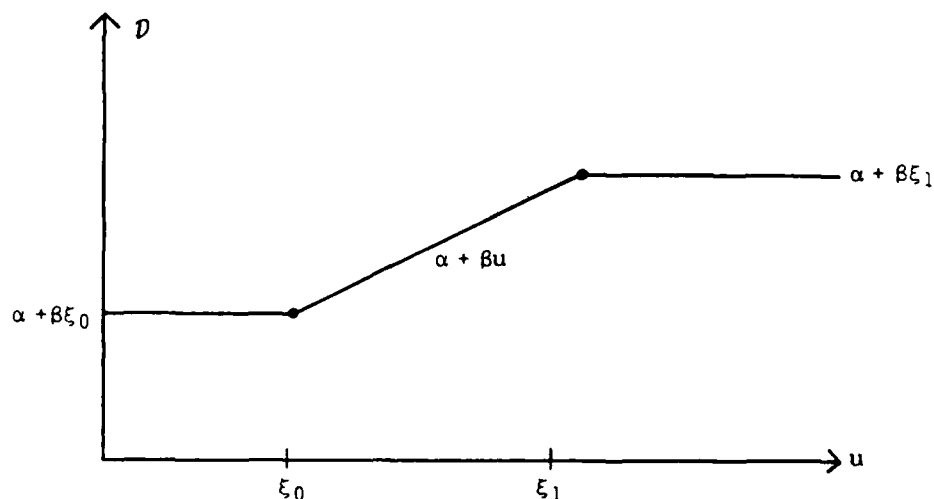


Figure 1

Such dispersal coefficients represent a rate that is bounded below and above (basal and saturation limits) and depends linearly on the density between these bounds. Problems with density-dependent dispersal have received attention elsewhere [28], [29] (see also [26] for further discussions regarding the importance of such problems).

Before using our estimation or inverse techniques in problems with experimental data, we carry out a rather careful testing of the methods with "synthetic" data on numerous examples. This procedure involves a series of tests using "data" generated (with noise) from a system with known (prechosen) parameters to ascertain the ability to recover the parameters from given sets of "data". For detailed explanations of this procedure, see for example [3], [5]. This testing is also combined with attempts to establish convergence and stability results for the methods. For problems involving systems of the type (3), such results are given in [1], [10], [11]. We present here results from two of the numerical tests we performed.

Example 1: We seek to estimate $D = D(u)$, i.e., ξ_0 , ξ_1 , α , β in Figure 1, in the system

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left[D(u) \frac{\partial u}{\partial x} \right] + 2u^2 - \frac{1}{2}u^3 + F(t, x), \quad u(t, 0) = u(t, 1) = 0, \quad u(0, x) = 6x(1-x),$$

where F is known (computed analytically so that $u(t, x) = 6x(1-x)(1+t^2)$ is a solution

corresponding to a "true" parameter D^* with $\xi_0=.5$, $\xi_1=1.6$, $\alpha=3$, $\beta=1$). "Data" corresponding to observations at (t_i, x_j) , $t_i=0,.5,1,x_j=.1,2,\dots,9$, were used for the inverse procedure. Results for estimation with $N=6$ and $N=14$ (cubic splines were used for the state approximations - see [10] for details) along with the initial estimate D^0 and true value D^* are depicted in Figure 2.

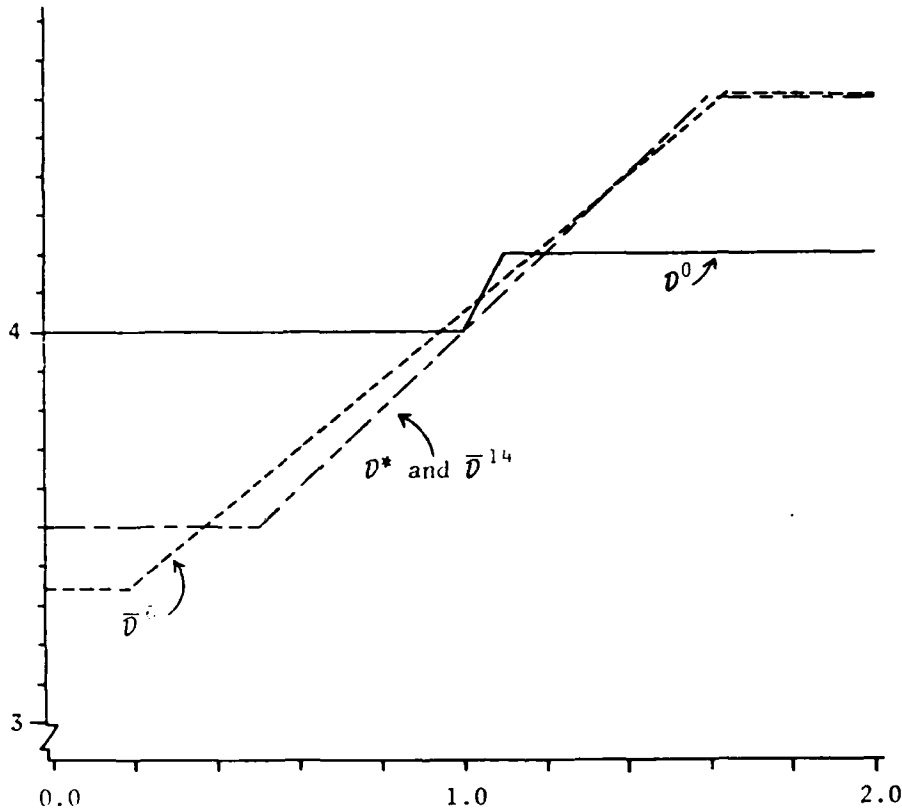


Figure 2

Example 2: We seek to estimate q and the nonlinearity f (we do not make any a priori parametrization or shape assumption on f) in

$$\frac{\partial u}{\partial t} = q \frac{\partial^2 u}{\partial x^2} + f(u) + F(t,x), \quad u(t,0) = u(t,1) = 0, \quad u(0,x) = 6x(1-x),$$

where again F is computed so that $u(t,x) = 6x(1-x)(1+t^2)$ is a solution corresponding to true values $q^* = 3.0$, $f^*(u) = 2u^2 - \frac{1}{2}u^3$. Results for the simultaneous estimation of f and q with state approximation $N=6$ (cubic splines with mesh $h = \frac{1}{6}$) and parameter approximations (linear splines) for f with mesh size $h=.65$ (see [11] for further details) are presented in Figure 3. These results for the initial estimate f^0 , the converged value $f^{6.65}$, and f^* correspond to initial guess $q^0=1.0$ and converged value $\bar{q}^6=2.9993$.

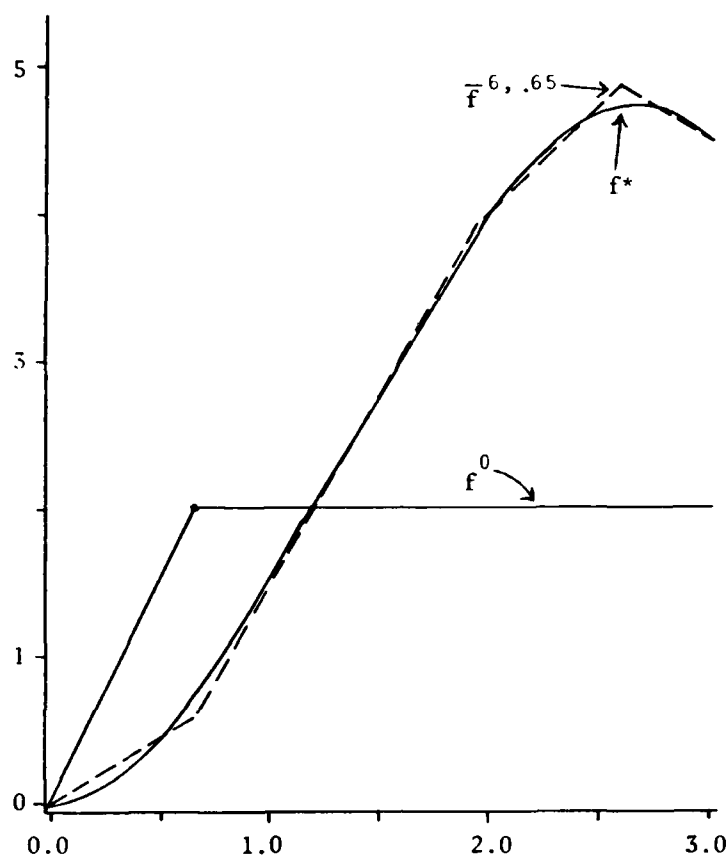


Figure 3

SIZE DEPENDENT GROWTH MODELS

We are currently using our parameter estimation techniques in investigations that entail size dependent population growth models. Data from experiments with mosquito fish populations in rice paddies have motivated our collaborative efforts with L. Botsford (U. California, Davis). While the basic problems we are considering are control problems for the mosquito fish/mosquito populations, a substantial effort is required in developing the underlying dynamics (i.e., growth models). For a more detailed description of the modeling and control problems, we refer to [17], [30].

A simple version of the basic modeling problem entails estimation of $q=(g,m,b)$ in the system

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} (gu) = -mu \quad x_0 \leq x \leq x_1, t > 0, \quad u(0,x) = \Phi(x), \quad g(x_0)u(t,x_0) = \int_{x_0}^{x_1} b(t,\xi)u(t,\xi)d\xi, \quad (4)$$

where g =growth rate, m =mortality rate, and b =fecundity are in general dependent on time t and size x , with x_0, x_1 the minimum and maximum observable sizes, respectively. Data for the system generally consists of observations that yield values $\hat{u}(t_i, x)$, $x_0 \leq x \leq x_1$, so that a distributed least-squares criterion, e.g.,

$$J(q) = \sum_i |u(t_i, \cdot; q) - \hat{u}(t_i, \cdot)|^2_{L^2}$$

is appropriate.

Since a convergence theory for the estimation problem has not appeared elsewhere, we sketch one approach to this problem. This approach is the analogue to that given in [1], [10], [11] for the insect dispersal model problems. We first rewrite (4) in variational or weak form. We seek $u(t) \in H^0(x_0, x_1)$ satisfying for all $\phi \in H^1(x_0, x_1)$

$$\langle u_t, \phi \rangle + \langle mu, \phi \rangle - \langle gu, D\phi \rangle - \phi(x_0)R(t, u) = 0, \quad u(0, \cdot) = \phi \quad (5)$$

where $R(t, \psi) \equiv \int_{x_0}^{x_1} b(t, \xi)\psi(\xi)d\xi$, $D = \frac{\partial}{\partial x}$, and $\langle \cdot, \cdot \rangle$ is the usual $L^2 = H^0$ inner product. For brevity, we assume that the parameters g and m depend only on size x . The ideas we present here can be readily modified to treat theoretically and computationally the more general case where g and m also are time dependent.

We assume that (g, m, b) are to be chosen from function spaces $G \times M \times B \subset H^1(x_0, x_1) \times H^0(x_0, x_1) \times H^0([0, T] \times [x_0, x_1])$ containing only nonnegative functions g, m, b where the functions in G also satisfy $g(x_1) = 0$ and $g(x_0) \geq \nu_1$ for some positive constant ν_1 . For the approximating systems (see [4], [10]) we assume that subspaces $Z^N \subset H^1(x_0, x_1)$ are chosen and let $u^N(t) \in Z^N$ denote solutions to

$$\langle u_t^N, \psi \rangle + \langle mu^N, \psi \rangle - \langle gu^N, D\psi \rangle - \psi(x_0)R(t, u^N) = 0, \quad \text{for all } \psi \in Z^N, \quad u^N(0) = P^N \phi, \quad (6)$$

where P^N is the orthogonal projection of $H^0(x_0, x_1)$ onto Z^N . We assume that the subspaces Z^N satisfy:

(H₁) For $\phi \in H^1$ we have $P^N \phi \rightarrow \phi$ in H^1 while for $\phi \in H^0$ we have $P^N \phi \rightarrow \phi$ in H^0 .

A number of the commonly used approximating families (piecewise linear, cubic splines [27]) satisfy this hypothesis. The ideas here can be slightly modified (see the remarks in [1]) to also include spectral families (such as Legendre polynomials - see [20]) in the state approximation schemes for which the convergence theory presented here is valid.

We further assume that G, M, B are compact in H^1, H^0, H^0 respectively, and that compact approximation families G^M, M^M, B^M for G, M, B respectively have been chosen satisfying:

(H₂) For $g^M \in G^M$, $g^M(x_1) = 0$, $g^M(x_0) \geq \nu_1$, $\|Dg^M\|_\infty \leq \mu_1$, and $G^M = i_1^M(G)$ where for each $g \in G$, $i_1^M(g) \rightarrow g$ in H^1 with the convergence uniform in $g \in G$;

(H₃) For $m^M \in M^M$, $\|m^M\|_\infty \leq \mu_2$, and $M^M = i_2^M(M)$ where for each $m \in M$, $i_2^M(m) \rightarrow m$ in H^0 with the convergence uniform in $m \in M$;

(H₄) For $b^M \in B^M$, $\|b^M(t, \cdot)\|_\infty \leq \mu_3$, and $B^M = i_3^M(B)$ where for each $b \in B$, $i_3^M(b) \rightarrow b$ in H^0 with the convergence uniform in $b \in B$.

We next remark that to give a convergence theory it suffices (see [8]) to argue that $u^N(t; q^M) \rightarrow u(t; q)$ in H^0 for each t as $N, M \rightarrow \infty$ whenever $\{q^M\}$ is an arbitrary sequence with $q^M \in G^M \times M^M \times B^M$ and $q^M \rightarrow q \in G \times M \times B$. Indeed, it suffices to give these arguments in the form $u^N(t; q^N) \rightarrow u(t; q)$ whenever $\{q^N\}$ is arbitrary in $G \times M \times B$ with $q^N \rightarrow q$ in $G \times M \times B$ (in the $H^1 \times H^0 \times H^0$ topology in this case). We sketch the arguments; let $\{q^N\}$ be arbitrary with $q^N \rightarrow q$ in $G \times M \times B$ and let $u^N(q^N)$, $u(q)$ be the solutions to (6), (5), respectively, corresponding to $q^N = (g^N, m^N, b^N)$.

$q=(g,m,b)$ respectively. From (H_1) , it suffices to argue that $z^N(t) \equiv u^N(t;q^N) - P^N u(t;q) \rightarrow 0$ in $H^0(x_0, x_1)$ for each t in $(0, T)$.

Letting $R^N(t, \psi) \equiv \int_{x_0}^{x_1} b^N(t, \xi) \psi(\xi) d\xi$, we have from (5) and (6) that for all $\phi \in Z^N$

$$\begin{aligned} \langle (u^N - P^N u)_t, \phi \rangle &= \langle u_t^N - u_t + (u - P^N u)_t, \phi \rangle \\ &= \langle (I - P^N) u_t, \phi \rangle + \langle \mu u - m^N P^N u, \phi \rangle + \langle g^N u^N - g u, D\phi \rangle + \phi(x_0) \Delta R^N \end{aligned}$$

where $\Delta R^N \equiv R^N(t, u^N) - R(t, u)$. With z^N as defined above we have $z^N(0) = 0$ and

$$\begin{aligned} \langle z_t^N, \phi \rangle &= \langle (I - P^N) u_t, \phi \rangle + \langle \mu u - m^N P^N u, \phi \rangle - \langle m^N z^N, \phi \rangle \\ &\quad + \langle g^N P^N u - g u, D\phi \rangle + \langle g^N z^N, D\phi \rangle + \phi(x_0) \Delta R^N. \end{aligned}$$

Choosing $\phi = z^N$ in this identity we find

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |z^N|^2 + \langle m^N z^N, z^N \rangle - \langle g^N z^N, D z^N \rangle \\ = \langle (I - P^N) u_t, z^N \rangle + \langle \mu u - m^N P^N u, z^N \rangle + \langle g^N P^N u - g u, D z^N \rangle + z^N(x_0) \Delta R^N. \end{aligned}$$

Recalling that $g^N(x_1) = g(x_1) = 0$, with integration by parts we find

$$\langle g^N z^N, D z^N \rangle = -\frac{1}{2} \langle D g^N z^N, z^N \rangle - \frac{1}{2} g^N(x_0) z^N(x_0)^2$$

and

$$\langle g^N P^N u - g u, D z^N \rangle = -\langle D(g^N P^N u - g u), z^N \rangle - [g^N P^N u - g u](x_0) z^N(x_0).$$

Hence, we have

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |z^N|^2 + \langle m^N z^N, z^N \rangle + \frac{1}{2} \langle D g^N z^N, z^N \rangle + \frac{1}{2} g^N(x_0) z^N(x_0)^2 \\ = \langle (I - P^N) u_t, z^N \rangle + \langle \mu u - m^N P^N u, z^N \rangle - \langle D(g^N P^N u - g u), z^N \rangle \\ + z^N(x_0) [(g u - g^N P^N u)(x_0) + \Delta R^N]. \end{aligned} \quad (7)$$

Using the bounds from (H_2) , (H_3) we find

$$\langle m^N z^N, z^N \rangle + \frac{1}{2} \langle D g^N z^N, z^N \rangle + \frac{1}{2} g^N(x_0) z^N(x_0)^2 \geq \mu |z^N|^2 + \nu z^N(x_0)^2$$

for positive constants μ, ν . Standard inequalities imply that the right side of the equality (7) is less than or equal to

$$\begin{aligned} \frac{1}{4\epsilon} \left\{ |(I - P^N) u_t|^2 + |\mu u - m^N P^N u|^2 + |D(g^N P^N u - g u)|^2 \right\} \\ + 3\epsilon |z^N|^2 + \epsilon |z^N(x_0)|^2 + \frac{1}{4\epsilon} \left\{ 2 |(g u - g^N P^N u)(x_0)|^2 + 2 |\Delta R^N|^2 \right\}, \end{aligned}$$

where $\epsilon > 0$ is arbitrarily chosen. From the bounds of (H_4) we have that $|R^N(t, z^N)| \leq k |z^N|$ and

defining $\delta^N(t) \equiv R^N(t, P^N u - u) + R^N(t, u) - R(t, u)$ we may conclude that

$$|\Delta R^N| \leq k |z^N| + |\delta^N(t)|.$$

Using these inequalities in (7) we obtain

$$\frac{1}{2} \frac{d}{dt} |z^N|^2 + \left[\mu - 3\epsilon - \frac{k^2}{\epsilon} \right] |z^N|^2 + (\nu - \epsilon) |z^N(x_0)|^2 \leq h^N(t) \quad (8)$$

where

$$h^N(t) \equiv \frac{1}{4\epsilon} \left\{ |(I - P^N)u_t|^2 + |\mu u - m^N P^N u|^2 + |D(g^N P^N u - gu)|^2 \right. \\ \left. + 2 |(gu - g^N P^N u)(x_0)|^2 + 4 |\delta^N(t)|^2 \right\}.$$

Choosing $\epsilon = \nu$ and using $z^N(0) = 0$, we may apply Gronwall's lemma to conclude that it suffices to argue that $h^N(t) \rightarrow 0$ in $L^1(0, T)$ to obtain the desired results. Under sufficient smoothness for $u(t)$, this follows readily from $(H_1) - (H_4)$.

While we are still testing our methods for use with models such as (4), our initial findings are quite positive. We present one of our simple test examples.

Example 3: We seek to estimate g in (4) with $m=2$, $b(x) = 12x\sqrt{1-x}$, $\Phi(x) = \sqrt{2}\sqrt{1-x}$, $x_0=0$, $x_1=1$. The solution corresponding to $g^*(x) = 2(1-x)$ is given by $u(t, x) = e^t \sqrt{2}\sqrt{1-x}$. Cubic splines (Z^N of dimension $N+3$) were used for the state approximations while linear splines (Q^M of dimension M) were used in parameter approximations $g^M(x) = \sum \alpha_i \hat{f}_i(x)$, where the sum is from $i=0$ to $i=M-1$ and \hat{f}_i is the usual "hat" function basis element [27] with support in $((i-1)/M, (i+1)/M)$. For $M=4$, the true value g^* corresponds to coefficients $g^* \sim (\alpha_0^*, \alpha_1^*, \alpha_2^*, \alpha_3^*) = (2.0, 1.5, 1.0, .5)$. Using data at eleven points in time and space each and initial guess $(1, 1, 1, 1)$, we obtained the converged values $(1.998, 1.498, 1.000, .496)$ for α -coefficients in the representation for $\bar{g}^{32,4}$, i.e., with $N=32$, $M=4$. The graphs of g^* and $\bar{g}^{32,4}$ are not distinguishable using ordinary plotting devices and hence we do not present them.

COMPUTATIONAL CONSIDERATIONS

The problems on which we have focused in this presentation are computationally intensive. Even simple examples such as those presented above can require from 10^2 to 10^4 seconds on an IBM 3081 and we are now using the ideas discussed here in research problems for which use of such a sequential machine would require rather prohibitive computational expenditures. The necessary software packages must deal with reasonably large vector/tensor systems and involve many repetitive routine calculations. Therefore, a substantial part of our research efforts over the last year have entailed development of ideas, algorithms, and software to take advantage of emerging computer architectures involving parallel and vector computational capabilities. Use of such architectures (in our research programs at Brown University and ICASE, we are currently employing a CRAY X-MP - a widely known vector machine - and a STAR ST-100 array processor with parallel features) has substantially enhanced

our efforts to investigate some of the research questions in modeling outlined above. For example, results for problems of the type given in Example 1 typically require from 10^3 to 10^4 seconds on the IBM 3081, but when the algorithms and corresponding software are modified to take advantage of the arithmetic speed and vector capabilities of the CRAY, we can carry out the same computational runs in 50 to 200 seconds on a CRAY X-MP.

Research machines such as the CRAY are, through NSF and other research sponsoring agencies, becoming readily accessible to many scientists in the U.S. We recognize that the machines we are presently using for these techniques and methods are not widely available to the world-wide biological research community. However, we firmly believe that the current revolution in computer hardware development has important implications for the community. We note that many of the high speed, parallel and vector features of large, expensive research array processors such as the FPS-164 and STAR ST-100 and research vector machines such as the CRAY X-MP (and 1-S) and CYBER 205 are rapidly becoming available in small, relatively inexpensive desk-top configurations. A number of attached array processor units and boards are now available for use with personal computers such as the IBM PC XT. Recently, new high speed chips (e.g., INTEL 80386 - a 32 bit, 4 MFLOPS chip) have been announced and will be available in PC's in 1987. We believe that the wide availability of "desk-top CRAY" capability discussed in the computer science community is only several years away. If we can successfully develop ideas further along the lines of those discussed above, the potential for a significant impact on biological modeling and research is enormous.

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